

Magnetic Exchange Interaction in the Spin Polarized Electron Gas

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(Dated: October 4, 2016)

The exchange interaction between two magnetic moments embedded in a host metal is fundamental to the description of the magnetic behavior of solids. In the standard spin-degenerate electron gas, it leads to the well known Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction, which is of the Heisenberg form $J\vec{S}_1 \cdot \vec{S}_2$, where the interaction strength J oscillates and falls off with the distance between the moments in a characteristic way. Here, we study the more general case of the spin-polarized electron gas both in two and three dimensions, by evaluating the interaction strength as an integration over the product of the host Green's functions. We find that in addition to the Heisenberg term, an additional Ising-like term appears in the magnetic interaction, so that the net interaction for the spin-polarized gas is of the form $J_1\vec{S}_1 \cdot \vec{S}_2 + J_2S_{1z}S_{2z}$. The interactions show a beating pattern as a function of distance, caused by the two different Fermi momenta for the two spins.

PACS numbers: 75.30.Hx, 75.30.Et, 71.70.Gm

I. INTRODUCTION

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction¹⁻³ is an indirect exchange interaction between two localized magnetic moments, mediated by electrons of the host crystal, and it has been extensively studied in one¹⁰, two¹¹, or three dimensions¹². For a system with no broken symmetry (inversion or time reversal), this interaction has the Heisenberg form of $E(\vec{R}) = J\vec{S}_1 \cdot \vec{S}_2$. For the standard free electron gas, J shows an oscillatory behavior as a function of the distance \vec{R} between the two moments, with the long-distance behavior $J(\vec{R}) \sim \cos(2k_F R)/R^d$, where k_F is the Fermi momentum and d is the dimensionality of the system. The recent observation of the skyrmions in solids¹³⁻¹⁶, caused due to the competition between RKKY and Dzyaloshinsky-Moriya (DM) interactions, originating from broken symmetry and spin-orbit interaction, has stimulated considerable interest in systems with broken symmetry.

The spin polarized electron gas, which we consider here, is the simplest example of a system with broken symmetry, and serves to illustrate the effect of the broken symmetry on the magnetic interaction. Time reversal and inversion symmetries lead, respectively, to the conditions for the band structure energies: $\varepsilon_{\vec{k}\uparrow} = \varepsilon_{-\vec{k}\downarrow}$ and $\varepsilon_{\vec{k}\uparrow} = \varepsilon_{-\vec{k}\uparrow}$. These conditions together lead to the spin-degenerate energies in the band structure, viz., $\varepsilon_{\vec{k}\uparrow} = \varepsilon_{\vec{k}\downarrow}$. Note that the spin-polarized electron gas has the inversion symmetry present, but the time reversal symmetry is broken.

Broken symmetries, break this degeneracy of the energy bands, change the Green's function matrix, and finally lead to extra terms in the interaction between two localized magnetic moments. Using lattice models, Dzyaloshinski and Moriya showed that^{18,19} in certain situations with broken inversion symmetry, the net interaction is given by the expression: $E(\vec{R}) = J(\vec{R})\vec{S}_1 \cdot \vec{S}_2 +$

$\vec{D}(\vec{R}) \cdot \vec{S}_1 \times \vec{S}_2 + \vec{S}_1 \cdot \vec{\Gamma} \cdot \vec{S}_2$, where in addition to the scalar RKKY-type interaction, we also have the vector and tensor interactions between the two localized moments \vec{S}_1 and \vec{S}_2 . For the spin-polarized electron gas discussed below, we will find that the scalar and tensor terms are non zero and their magnitudes are such that the net interaction may be written as

$$E(R) = J_1\vec{S}_1 \cdot \vec{S}_2 + J_2S_{1z}S_{2z}. \quad (1)$$

The DM vector interaction \vec{D} turns out to be zero, because the present system is inversion symmetric.

II. EXPRESSION FOR MAGNETIC INTERACTION

As usual, we take the localized moments to interact with the host electrons, described by the Hamiltonian \hat{H} , via the contact interaction

$$V_1(\vec{r}) = -\lambda \delta(\vec{r}) \vec{S}_1 \cdot \vec{s}, \quad (2)$$

and

$$V_2(\vec{r}) = -\lambda \delta(\vec{r} - \vec{R}) \vec{S}_2 \cdot \vec{s}, \quad (3)$$

where \vec{s} is the spin of the electron. Using the second-order perturbation theory, one can evaluate the interaction energy between the two localized spins. The result is

$$E(\vec{R}) = \frac{-\lambda^2}{\pi} \text{Im} \int_{-\infty}^{E_F} \text{Tr}[G(0, \vec{R}, E) \vec{S}_2 \cdot \vec{s} G(\vec{R}, 0, E) \vec{S}_1 \cdot \vec{s}] dE, \quad (4)$$

where $\hat{G}(E) = (E + i\mu - \hat{H})^{-1}$ with $\mu \rightarrow 0^+$, is the retarded Green's function. The matrix elements are given by

$$G_{\sigma_1\sigma_2}(\vec{r}_1, \vec{r}_2, E) = \sum_{\vec{k}\nu} \frac{\psi_{\vec{k}\nu}(\vec{r}_1, \sigma_1) \psi_{\vec{k}\nu}^*(\vec{r}_2, \sigma_2)}{E + i\mu - \varepsilon_{\vec{k}\nu}}, \quad (5)$$

where $G_{\sigma_1\sigma_2}(\vec{r}_1, \vec{r}_2, E) \equiv \langle \vec{r}_1\sigma_1 | \hat{G}(E) | \vec{r}_2\sigma_2 \rangle$, $\psi_{\vec{k}\nu}(\vec{r}, \sigma) = \langle \vec{r}\sigma | \vec{k}\nu \rangle$, and $\vec{k}\nu$ labels the eigenstates of the system.

The eigenstates are in general spin mixed, but in the present case they are spin pure states, so that the Green's function is diagonal in the spin indices. Furthermore, if the wave functions can be chosen to be real (true if $\psi_{\vec{k}\nu}(\vec{r}, \sigma)$ and $\psi_{\vec{k}\nu}^*(\vec{r}, \sigma)$ are solutions with the same energy), then it follows from Eq. (5) that $G_{\sigma_1\sigma_2}(\vec{r}_1, \vec{r}_2, E) = G_{\sigma_2\sigma_1}(\vec{r}_2, \vec{r}_1, E)$. In the present case, the Green's function being spin diagonal, we have the equality $G(0, \vec{R}, E) = G(\vec{R}, 0, E)$.

Under these conditions, we can expand the Green's function matrix in terms of $\vec{\sigma}$, the Pauli matrices as

$$G(0, \vec{R}, E) = G(\vec{R}, 0, E) = g_0(E)\sigma_0 + g_z(E)\sigma_z, \quad (6)$$

σ_0 being the unit 2×2 matrix. The energy expression Eq. 4 can be evaluated using the following spin identities

$$\begin{aligned} \text{Tr}[\vec{S}_2 \cdot \vec{\sigma} \vec{S}_1 \cdot \vec{\sigma}] &= 2\vec{S}_1 \cdot \vec{S}_2, \\ \text{Tr}[\vec{S}_2 \cdot \vec{\sigma} \sigma_z \vec{S}_1 \cdot \vec{\sigma}] &= 2i(\vec{S}_1 \times \vec{S}_2)_z, \\ \text{Tr}[\sigma_z \vec{S}_2 \cdot \vec{\sigma} \sigma_z \vec{S}_1 \cdot \vec{\sigma}] &= -2\vec{S}_1 \cdot \vec{S}_2 + 4S_{1z}S_{2z}. \end{aligned} \quad (7)$$

The result is

$$E(\vec{R}) = J_1\vec{S}_1 \cdot \vec{S}_2 + J_2S_{1z}S_{2z}, \quad (8)$$

where

$$\begin{aligned} J_1 &= \frac{-\lambda^2\hbar^2}{2\pi} \times \text{Im} \int_{-\infty}^{E_F} (g_0^2 - g_z^2) dE, \\ J_2 &= \frac{-\lambda^2\hbar^2}{2\pi} \times \text{Im} \int_{-\infty}^{E_F} 2g_z^2 dE. \end{aligned} \quad (9)$$

These expressions can be evaluated from the Green's functions, which we now proceed to do for the spin-polarized electron gas in 2D and 3D. Note from Eq. 9 that for the standard (spin unpolarized) electron gas, the Green's function has equal diagonal elements, so that $g_z = 0$, and the J_2 terms vanishes as a result and one obtains the standard $\vec{S}_1 \cdot \vec{S}_2$ RKKY interaction.

III. SPIN POLARIZED ELECTRON GAS IN 3D

Our starting point is the electron band structure

$$\varepsilon_{\vec{k}\sigma} = \frac{\hbar^2 k^2}{2m} \mp \Delta, \quad (10)$$

where $-(+)$ sign is for spin up (down) states, so that 2Δ is the band splitting between the up- and down-spin states. The corresponding plane-wave eigenstates are

$$|\vec{k}\sigma\rangle = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}} |\sigma\rangle, \quad (11)$$

where the Ω is the volume of the box for normalization. The key quantity to evaluate is the Green's function,

which, using Eqs. (5), (10), and (11) and converting the summation into integration in the momentum space, is written as

$$G_{\sigma\sigma'}(\vec{r}, \vec{r}', E) = \frac{\delta_{\sigma\sigma'}}{(2\pi)^3} \int \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{E + i\eta - \varepsilon_{\vec{k}\sigma}} d^3k. \quad (12)$$

The integral can be evaluated by a straightforward contour integration^{12,20} to yield the result

$$\begin{aligned} G(\vec{r}_1, \vec{r}_2, E) &= \begin{pmatrix} g_{\uparrow} & 0 \\ 0 & g_{\downarrow} \end{pmatrix} \\ &= \frac{-m}{2\pi r \hbar^2} \begin{pmatrix} e^{i\alpha(E+\Delta)r} & 0 \\ 0 & e^{i\alpha(E-\Delta)r} \end{pmatrix}, \end{aligned} \quad (13)$$

where $r \equiv |\vec{r}_1 - \vec{r}_2|$ and

$$\alpha(x) = \begin{cases} (2m\hbar^{-2}x)^{1/2} & \text{if } x > 0, \\ i(2m\hbar^{-2}|x|)^{1/2} & \text{if } x < 0. \end{cases} \quad (14)$$

The coefficients g_0 and g_z in Eq. (6) are then $g_0 = (g_{\uparrow} + g_{\downarrow})/2$ and $g_z = (g_{\uparrow} - g_{\downarrow})/2$, which are complex numbers.

Plugging these into Eq. (9) and performing the energy integrations, we find that the imaginary part vanishes, as it must, and the results for the magnetic interaction terms are given by

$$\begin{aligned} J_1 &= \frac{-\lambda^2 m^2}{8\pi^3 \hbar^2 R^2} \times \left(\int_{\Delta}^{E_F} \sin[k_+(E)R + k_-(E)R] dE \right. \\ &\quad \left. + \int_{-\Delta}^{\Delta} \exp[-\kappa(E)R] \times \sin[k_+(E)R] dE \right), \\ J_2 &= I(k_{F-}R) + I(k_{F+}R) - J_1, \end{aligned} \quad (15)$$

where E_F is the Fermi energy, $k_{\pm}(E) = [2m\hbar^{-2}(E \pm \Delta)]^{1/2}$ is the momentum for the spin up (down) state, $k_{F\pm} \equiv k_{\pm}(E_F)$ is the corresponding Fermi momentum for spin up (down) electrons, $\kappa(E) = [2m\hbar^{-2}(\Delta - E)]^{1/2}$, and

$$I(x) = -\frac{\lambda^2 m}{(4\pi)^3 R^4} \times [\sin(2x) - 2x \cos(2x)]. \quad (16)$$

The integral $I(x)$ is familiar from the theory of the spin-unpolarized electron gas, in which case, the RKKY interaction is, simply,

$$J_1 = 2I(k_F R), \quad (17)$$

$k_F = (2m\hbar^{-2}E_F)^{1/2}$ being the Fermi momentum. The results agree with our earlier work, where we had used a different method²⁰.

Note that if there is no spin polarization ($\Delta = 0$), then Eq. (15) immediately reduces to the expression Eq. (17) for the spin-unpolarized gas and $J_2 = 0$. The computed results for J_1 and J_2 , for the case of iron, are shown in Fig. 1, which show the oscillatory behavior characteristic of the inverse momentum $(k_{F+} + k_{F-})^{-1}$, and the beat pattern for J_2 is characteristic of the inverse difference

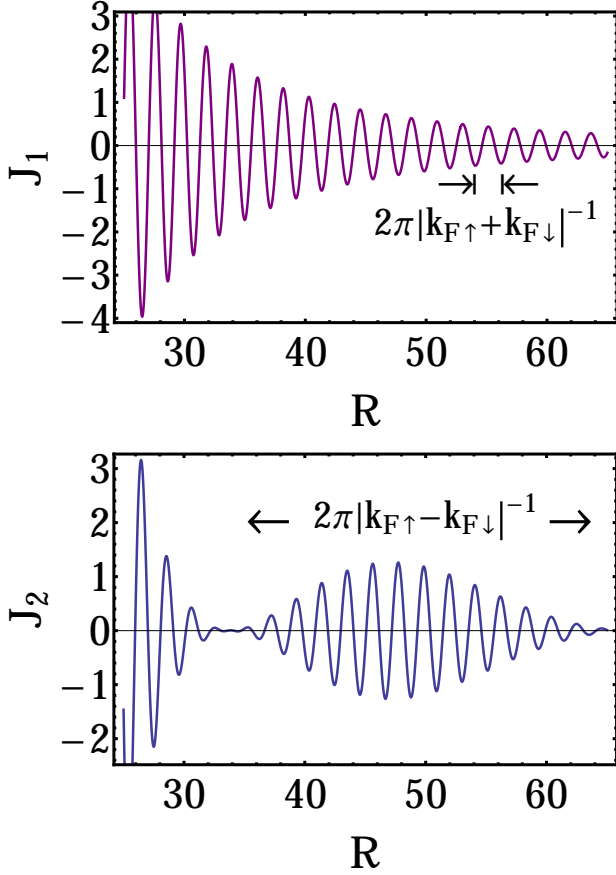


FIG. 1. Oscillatory behavior of J_1 and J_2 , in the units of $10^{-5}m\lambda^2\pi^{-3}$ as a function of R in the units of \AA for the case of iron.

$(k_{F+} - k_{F-})^{-1}$, respectively. Band calculations for iron²¹ lead to the $E_F \approx 8$ eV and $2\Delta \approx 2$ eV. One can use these values to find the Fermi momenta, $k_{F\uparrow} \simeq 1.574$ and $k_{F\downarrow} \simeq 1.388$ $1/\text{\AA}$. For long distances, we predict the oscillation periods to be: $2\pi|k_{F\uparrow} + k_{F\downarrow}|^{-1} \simeq 2.12$ \AA and for the beat pattern behavior $2\pi|k_{F\uparrow} - k_{F\downarrow}|^{-1} \simeq 33.75$ \AA . Fig. 1 shows a very good match between the computed results and predictions.

Discussions – An interesting situation occurs if $J_1 + J_2 = 0$, which can happen for certain distances. In this case, the net interaction, has the form of $E(\vec{R}) = J_1(S_{1x}S_{2x} + S_{1y}S_{2y})$, which would clearly align the spins in the xy -plane, i. e., normal to the spin polarization axis. In general, depending on the relative strengths of $J_1(\vec{R})$ and $J_2(\vec{R})$, the net spin interaction could align the two spins in different directions, leading to the possibility for unusual spin textures.

Note that apart from the position dependent interaction $E(\vec{R})$, there is a constant energy shift

$$E_0 = \frac{-\hbar\lambda}{12\pi^2}(S_{1z} + S_{2z})(k_{F+}^3 - k_{F-}^3), \quad (18)$$

a new term not present in the standard, non-spin-

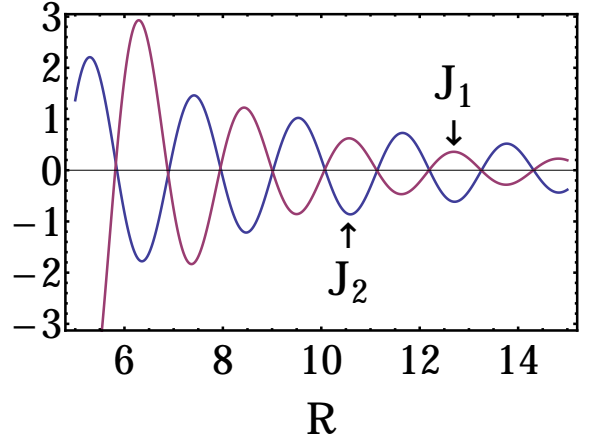


FIG. 2. Oscillatory behavior of J_1 and J_2 , in the units of $10^{-3}m\lambda^2\pi^{-3}$ as a function of R in the units of \AA for the case of iron.

polarized electron gas, and a term that tends to align the embedded spins \vec{S}_1 and \vec{S}_2 along the \hat{z} axis. This expression²⁰, obtained by using the first-order perturbation theory for the perturbing potentials, Eqs. (2) and (??), depends on the strength of the polarization of the electron gas and would dominate for strong spin polarization. In turn, for weak spin polarization ($\delta k_F \equiv k_{F+} - k_{F-} \ll m\lambda k_F^2/(Rk_F)^4$, where $k_F \equiv (k_{F+} + k_{F-})/2$), this term is negligible and the J_1 and J_2 interactions dominate.

Another point to note is that the essential ingredient for the presence of the DM interactions is the broken symmetry (time reversal or inversion or both). In the original DM work¹⁹, the spin-orbit coupling (SOC) provided the mechanism for the magnetic interaction. The interaction between the magnetic moments of two atoms occurred via an intermediate atom and involved the spin-orbit coupled excited states on the two atoms. In this case, as originally showed by DM, $J \sim \xi^0$, $\vec{D} \sim \xi$, and $\vec{\Gamma} \sim \xi^2$, where ξ is the spin-orbit coupling strength ($\xi \vec{L} \cdot \vec{S}$), so that $|\vec{\Gamma}| \ll |\vec{D}| \ll |J|$, ξ being a small parameter, and it is then customary to ignore the tensor DM interaction $\vec{\Gamma}$. In the present case, the broken time-reversal symmetry without the involvement of any SOC leads to the DM interaction, so that it is entirely a different mechanism, and further that the strengths of all terms are comparable, being proportional to λ^2 . Thus, in a solid, if a spin-polarized electron gas is present in addition to magnetic moments on atoms with SOC, both effects must be considered separately and the dominant effect for the DM interactions might as well come from the spin polarization of the electron gas, of the type studied in this paper.

IV. SPIN POLARIZED ELECTRON GAS IN 2D

The Green's function for the spin polarized electron gas in 2D is given by

$$G_{\sigma\sigma'}(\vec{r}, \vec{r}', E) = \frac{\delta_{\sigma\sigma'}}{(2\pi)^2} \int \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{E + i\eta - \varepsilon_{\vec{k}\sigma}} d^2k. \quad (19)$$

This is a standard integration, which can be evaluated by using the Jacobi-Anger expansion of the exponential term in terms of the Bessel's functions and by performing the angular integration.^{20,23,24} The result is

$$G_{\sigma\sigma}(\vec{r}, \vec{r}', E) = -\frac{m}{\pi\hbar^2} K_0 \left[-i \frac{\sqrt{2m}}{\hbar} |\vec{r} - \vec{r}'| \alpha(E \pm \Delta) \right], \quad (20)$$

where $+$ ($-$) is for $\sigma = \uparrow$ (\downarrow), K_0 is the modified Bessel function of the second kind, and

$$\alpha(x) = \begin{cases} \sqrt{x} & \text{if } x > 0, \\ i\sqrt{|x|} & \text{if } x < 0. \end{cases} \quad (21)$$

To find the imaginary and the real parts of the modified Bessel function, it is convenient to use the equality $K_\nu(x) = 2^{-1}\pi i^{\nu+1}H_\nu^1(ix)$, which is valid for $-\pi < \arg(x) \leq \pi/2$. The Hankel function of the first kind is written in terms of the Bessel and Neumann functions as $H_\nu^1(x) = J_\nu(x) + iY_\nu(x)$. The expansion coefficients for the Green's function, Eq. (6), are then $g_0 = 2^{-1}(G_{\uparrow\uparrow}(\vec{r}, \vec{r}', E) + G_{\downarrow\downarrow}(\vec{r}, \vec{r}', E))$ and $g_z = 2^{-1}(G_{\uparrow\uparrow}(\vec{r}, \vec{r}', E) - G_{\downarrow\downarrow}(\vec{r}, \vec{r}', E))$. Plugging these into Eq. (9), we find the results

$$\begin{aligned} J_1 &= \frac{\lambda^2 m^2}{8\pi\hbar^2} \left\{ -\frac{2}{\pi} \int_{-\Delta}^{\Delta} \text{Re}[K_0(\kappa R)] J_0(k_+ R) dE \right. \\ &\quad \left. + \int_{\Delta}^{E_F} [J_0(k_- R) Y_0(k_+ R) + Y_0(k_- R) J_0(k_+ R)] dE \right\}, \\ J_2 &= \frac{\lambda^2 m}{16\pi R^2} [I'(k_F - R) + I'(k_F + R)] - J_1, \end{aligned} \quad (22)$$

where $I'(x) = x^2[J_0(x)Y_0(x) + J_1(x)Y_1(x)]$.

In this case, similar to the case of 3D spin-polarized electron gas, the oscillatory behaviors of J_1 and J_2 show beat-pattern, caused by the two different Fermi momenta for the two spin channels.

V. SUMMARY

In this paper, we obtained the magnetic interactions between two localized moments, embedded in the spin polarized electron gas in two and three dimensions, extending the standard results for the spin-unpolarized electron gas, which leads to the well known RKKY interaction. The spin-polarization leads to an anisotropic Heisenberg type of interaction, of the form $J_1 \vec{S}_1 \cdot \vec{S}_2 +$

$J_2 S_{1z} S_{2z}$. Both terms J_1 and J_2 show oscillatory behavior as a function of distance between the two magnetic moments with the period of the oscillations determined by $\bar{k}_F R$, \bar{k}_F being the average Fermi momentum of the two spin channels and, in addition, J_2 shows a beating pattern determined by the momentum difference $k_{F+} - k_{F-}$. This is the simplest system with broken symmetry and serves to illustrate the origin of the magnetic interactions in the solid that go beyond the standard RKKY $\vec{S}_1 \cdot \vec{S}_2$ type interaction.

VI. ACKNOWLEDGMENTS

This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-00ER45818.

VII. APPENDIX

In this Appendix, we derive the general expression for the magnetic interaction, Eq. (4), from the second order perturbation theory, which is somewhat more pedagogical than found in the literature.

Let $\psi_{\vec{k}\nu}(\vec{r}\sigma)$ denote the host electron wave functions ($|\vec{k}\nu\rangle = \sum_{\vec{r}\sigma} \psi_{\vec{k}\nu}(\vec{r}\sigma) |\vec{r}\sigma\rangle$ in Dirac notations), where $k\nu$ are the quantum numbers (e. g., Bloch momentum k and band index ν in a crystal) and $\varepsilon_{k\nu}$ be the corresponding eigenenergies. The interaction between the two localized moments \vec{S}_1 and \vec{S}_2 (located at origin and \vec{R} , respectively) and the host electrons are taken, as usual, to be the contact interactions: $V_1(\vec{r}) = -\lambda \delta(\vec{r}) \vec{S}_1 \cdot \vec{s}$ and $V_2(\vec{r}) = -\lambda \delta(\vec{r} - \vec{R}) \vec{S}_2 \cdot \vec{s}$. According to the second-order perturbation theory, the change of energy due to this interaction is given by the equation

$$E(\vec{R}) = \sum_{\vec{k}\nu} \sum_{\vec{k}'\nu'}' \frac{|\langle \vec{k}\nu | \hat{V}_1 + \hat{V}_2 | \vec{k}'\nu' \rangle|^2}{\varepsilon_{\vec{k}\nu} - \varepsilon_{\vec{k}'\nu'}}, \quad (23)$$

where the prime over the summation indicates that the term $k'\nu' = k\nu$ is excluded and the interactions are in the operator forms, viz., $\hat{V}_1(\vec{r}) = -\lambda \sum_{\sigma\sigma'} |\vec{0}\sigma\rangle \vec{S}_1 \cdot \vec{s} \langle \vec{0}\sigma'|$ and $\hat{V}_2(\vec{r}) = -\lambda \sum_{\sigma\sigma'} |\vec{R}\sigma\rangle \vec{S}_2 \cdot \vec{s} \langle \vec{R}\sigma'|$. It is convenient to write the energy expression Eq. (23) in terms of the retarded and advanced Green's functions, $\hat{G}(E) = (E + i\mu - \hat{H})^{-1}$ and $\hat{G}^A(E) = (E - i\mu - \hat{H})^{-1}$, where $\mu \rightarrow 0^+$. With the use of the identity

$$P\left(\frac{1}{x}\right) = \lim_{\mu \rightarrow 0^+} \frac{1}{2} \left(\frac{1}{x + i\mu} + \frac{1}{x - i\mu} \right), \quad (24)$$

where P denotes the principal part, and the expression for the Green's function

$$\hat{G}(E) = \sum_{\vec{k}\nu} \frac{|\vec{k}\nu\rangle \langle \vec{k}\nu|}{E - \varepsilon_{\vec{k}\nu} + i\mu}, \quad (25)$$

one finds after some algebra, the result

$$E(\vec{R}) = \sum_{\vec{k}\nu}^{\text{occ}} \langle \vec{k}\nu | \hat{V}_2 \hat{G}(\varepsilon_{\vec{k}\nu}) \hat{V}_1 | \vec{k}\nu \rangle + h.c., \quad (26)$$

where the extra terms ($\vec{k}'\nu' = \vec{k}\nu$) added to Eq. (23) to write in terms of the Green's functions add up to zero. Note that only the cross terms in the interactions \hat{V}_1 and \hat{V}_2 have been kept, since only these depend on \vec{R} . Using the completeness relation $\sum_{\vec{r}\sigma} |\vec{r}\sigma\rangle \langle \vec{r}\sigma| = 1$, Eq. (26) can be expressed in terms of the real space wave functions

$$E(\vec{R}) = \lambda^2 \sum_{\vec{k}\nu}^{\text{occ}} \sum_{\sigma_1 \sigma_2} \langle \sigma_1 | \vec{S}_2 \cdot \vec{s} G(\vec{R}, 0, \varepsilon_{\vec{k}\nu}) \vec{S}_1 \cdot \vec{s} | \sigma_2 \rangle \times \psi_{\vec{k}\nu}^*(\vec{R}, \sigma_1) \psi_{\vec{k}\nu}(0, \sigma_2) + h.c., \quad (27)$$

where $G_{\sigma_1 \sigma_2}(\vec{r}_1, \vec{r}_2, E) \equiv \langle \vec{r}_1 \sigma_1 | \hat{G}(E) | \vec{r}_2 \sigma_2 \rangle$ is given by

$$G_{\sigma \sigma'}(\vec{r}_1, \vec{r}_2, E) = \sum_{\vec{k}\nu} \frac{\psi_{\vec{k}\nu}(\vec{r}_1, \sigma) \psi_{\vec{k}\nu}^*(\vec{r}_2, \sigma')}{E + i\mu - \varepsilon_{\vec{k}\nu}}. \quad (28)$$

Expressing the Green's function as an integral over energy

$$G(\vec{R}, 0, \varepsilon_{\vec{k}\nu}) = \int G(\vec{R}, 0, E) \delta(E - \varepsilon_{\vec{k}\nu}) dE, \quad (29)$$

and the fact that $\int_{-\infty}^{\infty} dE \times \sum_{\vec{k}\nu} \rightarrow \int_{-\infty}^{E_F} dE \times \sum_{\vec{k}\nu}^{\text{occ}}$, Eq. (27) leads to the result

$$E(\vec{R}) = \lambda^2 \int_{-\infty}^{E_F} dE \sum_{\sigma_1 \sigma_2} \langle \sigma_1 | \vec{S}_2 \cdot \vec{s} G(\vec{R}, 0, E) \vec{S}_1 \cdot \vec{s} | \sigma_2 \rangle \times \sum_{\vec{k}\nu} \psi_{\vec{k}\nu}^*(\vec{R}, \sigma_1) \psi_{\vec{k}\nu}(0, \sigma_2) \delta(E - \varepsilon_{\vec{k}\nu}) + h.c. \quad (30)$$

The second line can be expressed as the difference between the retarded and the advanced Green's function, viz.,

$$\begin{aligned} & \sum_{\vec{k}\nu} \psi_{\vec{k}\nu}^*(\vec{R}, \sigma_1) \psi_{\vec{k}\nu}(0, \sigma_2) \delta(E - \varepsilon_{\vec{k}\nu}) \\ &= \frac{i}{2\pi} [G(0, \vec{R}, E) - G^A(0, \vec{R}, E)]_{\sigma_2 \sigma_1}, \end{aligned} \quad (31)$$

since $\lim_{\mu \rightarrow 0^+} (x \pm i\mu)^{-1} = P(x^{-1}) \mp i\pi\delta(x)$, so that

$$\delta(E - \varepsilon_{\vec{k}\nu}) = \frac{i}{2\pi} \left(\frac{1}{E + i\mu - \varepsilon_{\vec{k}\nu}} - \frac{1}{E - i\mu - \varepsilon_{\vec{k}\nu}} \right). \quad (32)$$

From Eqs. (30) and (31), we find the final result

$$E(\vec{R}) = \frac{-\lambda^2}{\pi} \text{Im} \int_{-\infty}^{E_F} \text{Tr} [G(0, \vec{R}, E) \vec{S}_2 \cdot \vec{s} G(\vec{R}, 0, E) \vec{S}_1 \cdot \vec{s}] dE, \quad (33)$$

We left out here in Eq. (33), the term involving G^A , which turns out to be zero, i. e.,

$$I = \frac{\lambda^2}{\pi} \text{Im} \int_{-\infty}^{E_F} \text{Tr} [G^A(0, \vec{R}, E) \vec{S}_2 \cdot \vec{s} G(\vec{R}, 0, E) \vec{S}_1 \cdot \vec{s}] dE = 0. \quad (34)$$

This can be easily shown by expanding the Green's functions in terms of the Pauli matrices

$$\begin{aligned} G(\vec{R}, 0, E) &= g_0 \sigma_0 + \sum_{i=1}^3 g_i \sigma_i, \\ G^A(0, \vec{R}, E) &= g_0^* \sigma_0 + \sum_{i=1}^3 g_i^* \sigma_i, \end{aligned} \quad (35)$$

using the result $\text{Tr}(A + B) = \text{Tr} A + \text{Tr} B$ and the trace equalities

$$\begin{aligned} \text{Tr}(\sigma_i \sigma_j) &= 2\delta_{ij}, \\ \text{Tr}(\sigma_i \sigma_j \sigma_k) &= 2i \varepsilon_{ijk}, \\ \text{Tr}(\sigma_i \sigma_j \sigma_k \sigma_l) &= 2(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \end{aligned} \quad (36)$$

written in terms of the Kronecker deltas δ_{ij} and the Levi-Civita symbols ε_{ijk} .

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